COMSOL 2014

Full System Modeling and Validation of the Carbon Dioxide Removal Assembly

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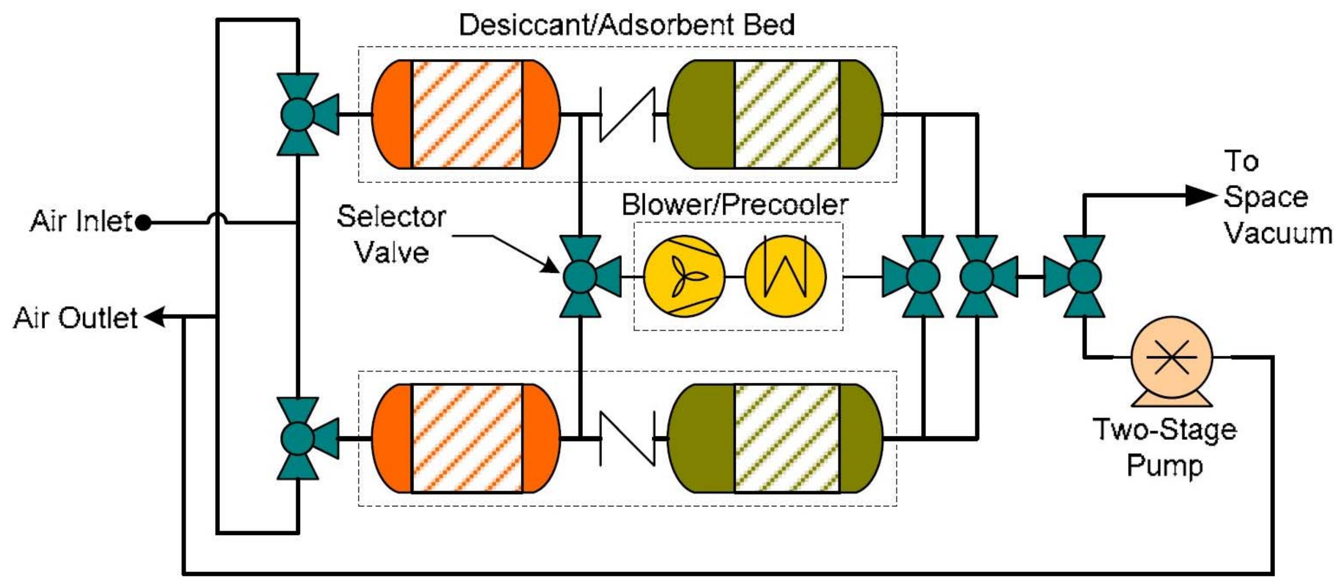
Robert Coker and Jim Knox

NASA Marshall Space Flight Center, Huntsville, Alabama, 35812, USA

Introduction

- Advanced Exploration Systems (AES) Program:
  - pioneering approaches for rapidly developing prototype systems
  - validating concepts for human missions beyond Earth orbit
- Atmosphere Resource Recovery and Environmental Monitoring Project (ARREM):
  - mature environmental subsystems
  - ***derived directly from the ISS subsystem architecture***
  - reduce developmental and mission risk
  - demonstrate concepts for human missions beyond Earth orbit

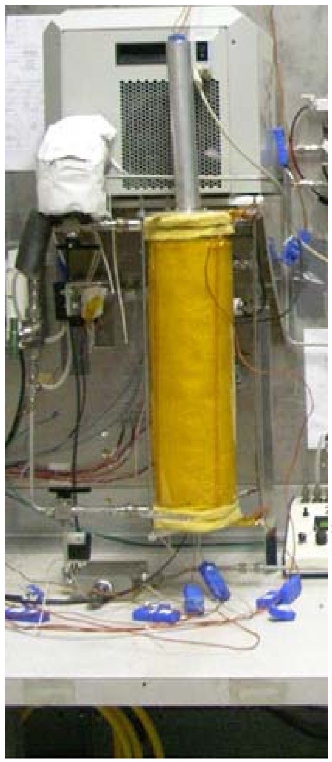
- Goal: *Predictive* model of the Carbon Dioxide Removal Assembly (CDRA)
- Here, focus on the Desiccant Beds (1D)
- Need to know sorbent behavior (isotherms, LDF, etc.)

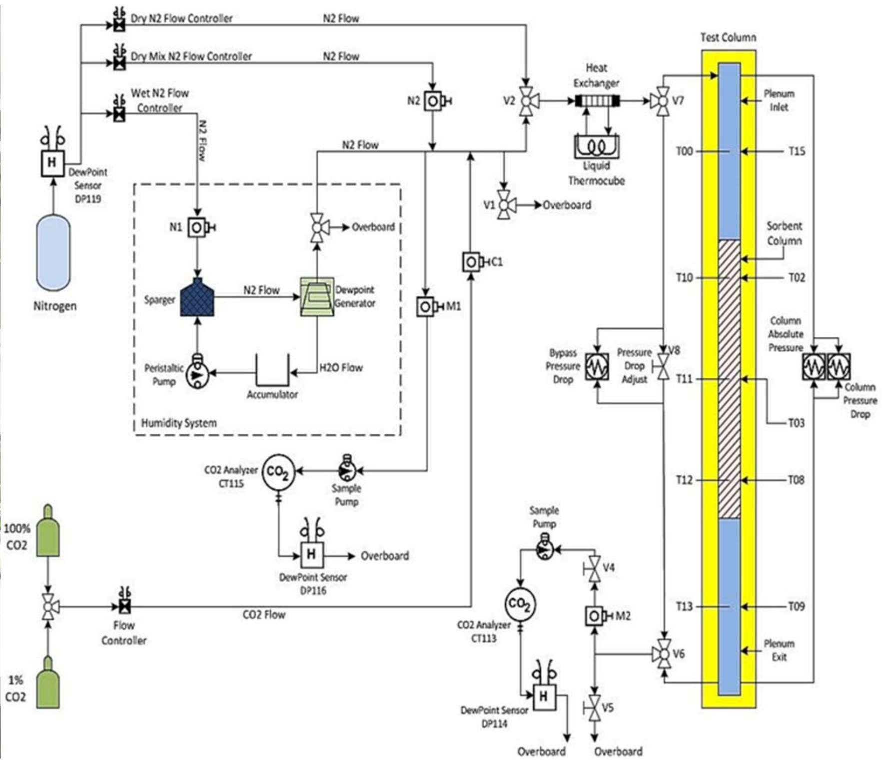


Cylindrical Breakthrough Test (CBT)

- Multiple sorbents: RK38, 13X G544, 5A G522, SG G40, SG B152
- Multiple sorbates: CO_2, H_2O
- Variable flow rates, concentrations, and temperatures

- Well diagnosed (TCs, FCs, DPs, PTs, masses)
- Insulated
- Surrogate for CDRA DBs





Model Approach

- Use Toth isotherms from other work
- Use dimensionless correlations (Re, Nu, Pe, Pr, Sc)
  - Derives mass dispersion and thermal transfer coefficients
- Assume binary mass diffusion is valid
- Assume constant porosity
- Use Rumpf-Gupte permeability relationship
- 1D ‘plug flow’ style model with wall corrections
- Fit the single remaining model parameter using CBT data
  - Across-the-board validity of the 1D LDF model?

COMSOL Model

Use COMSOL Multiphysics to solve 7 PDEs:

- 1^{st} order Ergun equation for interstitial velocity
- Gas pressure assuming ideal gas law
- Sorbate concentration via diffusion & advection
- Pellet loading via LDF & Toth
- Sorbent temperature with sorption physics
- Gas temperature (not in eqlbrm with sorbent)
- Wall housing temperature

- BCs tricky in COMSOL (applied only to flux terms)
- Time-dependent inlet conditions (flow rate, T_{gas}, concentration)
- Temperature-dependent material properties
- Adsorption and Desorption half-cycles with changing BCs

1-D Model PDEs

$$\rho_g \frac{\partial u}{\partial t} - \frac{\partial}{\partial x}\left(\frac{\mu_g}{\epsilon}\frac{\partial(\epsilon u)}{\partial x}\right) = -\left(\frac{\partial P}{\partial x} + u\left(\frac{\epsilon\mu_g}{\kappa} + \epsilon^2|u|\rho_g A + \frac{\partial q}{\partial t}\frac{(1-\epsilon)}{\epsilon}M_a + \rho_g\frac{\partial u}{\partial x}\right)\right)$$

$$\frac{\epsilon}{R_s T_g}\frac{\partial P}{\partial t} + \frac{\partial}{\partial x}\left(\frac{\epsilon u P}{R_s T_g}\right) + P\frac{\partial\left(\frac{\epsilon}{R_s T_g}\right)}{\partial t} = -\frac{\partial q}{\partial t}(1-\epsilon)M_a$$

$$0 = \epsilon\frac{\partial c}{\partial t} + (1-\epsilon)\frac{\partial q}{\partial t} + \frac{\partial}{\partial x}\left(-D_x\frac{\partial c}{\partial x} - D_x\frac{c}{M_{mix}}\frac{\partial M_{mix}}{\partial x} + D_x\frac{c}{\rho_g}\frac{\partial \rho_g}{\partial x} + u\epsilon c\right)$$

LDF parameter

$$\frac{\partial q}{\partial t} = (q_* - q)k_m$$

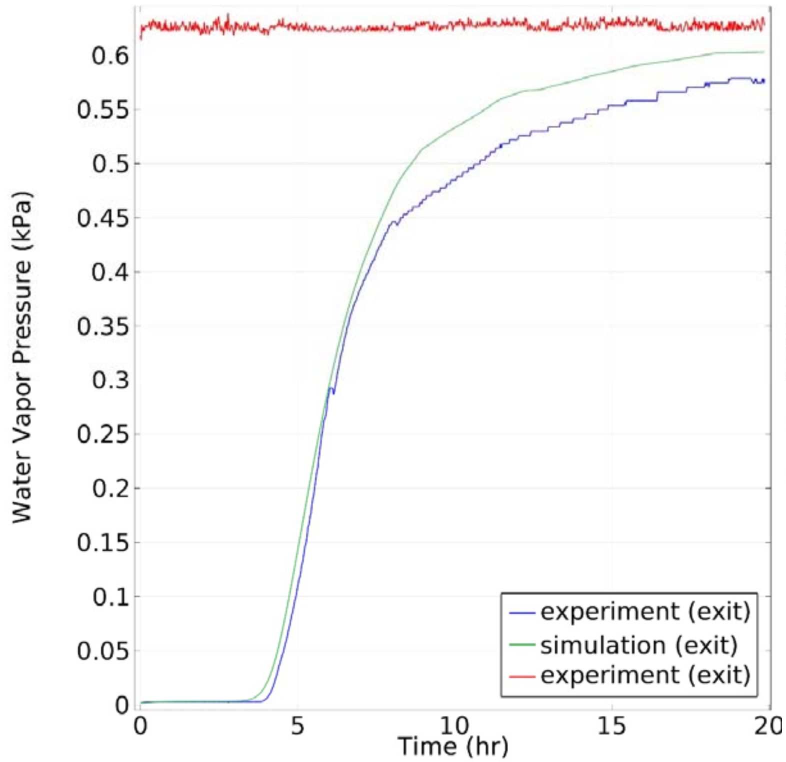
$$(1-\epsilon)\rho_s c_{ps}\frac{\partial T_s}{\partial t} + \frac{\partial}{\partial x}\left(-k_s(1-\epsilon)\frac{\partial T_s}{\partial x}\right) = \mathrm{A}h_{sg}\left(T_g - T_s\right) - \partial\mathrm{H}(1-\epsilon)\frac{\partial q}{\partial t}$$

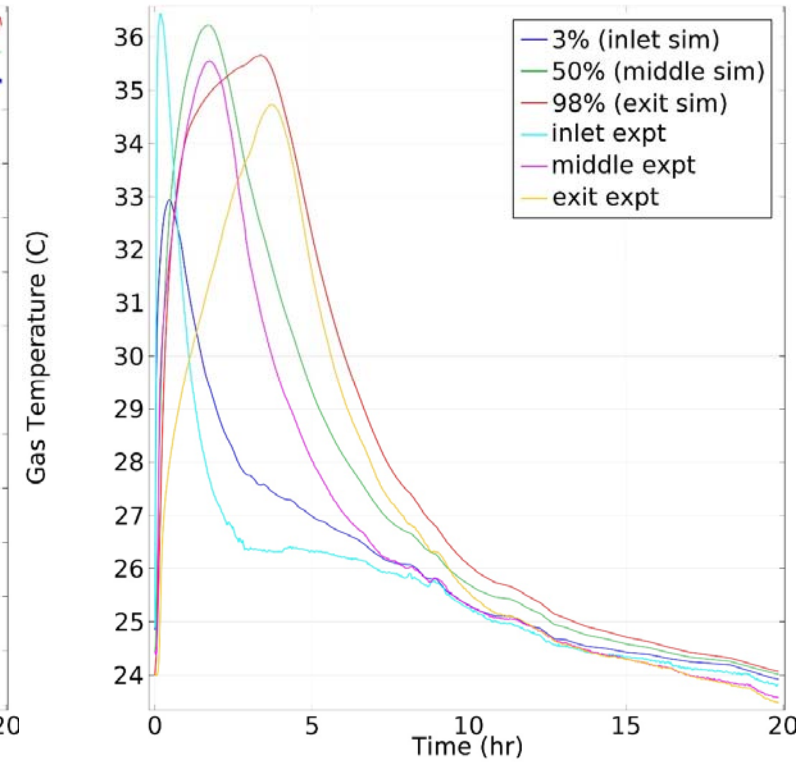
$$\epsilon\rho_g c_{pg}\frac{\partial T_g}{\partial t} + \frac{\partial}{\partial x}\left(-k_{gx}\epsilon\frac{\partial T_g}{\partial x}\right) = \mathrm{A}h_{sg}\left(T_s - T_g\right) - \epsilon\rho_g c_{pg} u\frac{\partial T_g}{\partial x} + \frac{P_I h_{gc}\left(T_c - T_g\right)}{A_f}$$

$$\rho_c c_{pc}\frac{\partial T_c}{\partial t} + \frac{\partial}{\partial x}\left(-k_c\frac{\partial T_c}{\partial x}\right) = \frac{P_I h_{gc}\left(T_g - T_c\right)}{A_c} + \frac{P_O h_{Ac}(T_A - T_c)}{A_c}$$

Example H_2O SG CBT Results

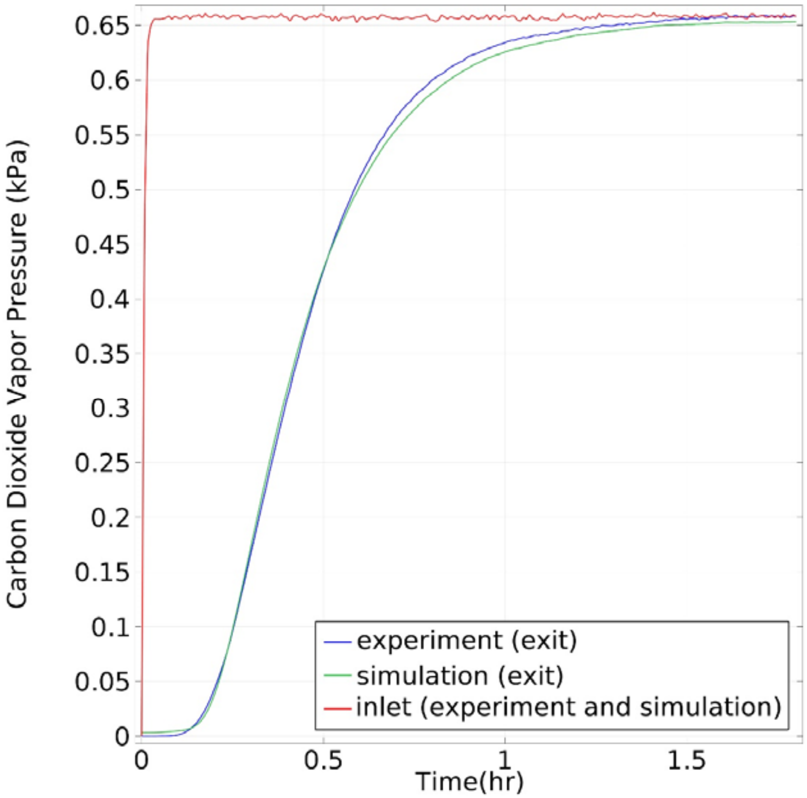
- Water vapor on Silica Gel Grade 40
- Flow is at 8 SLPM with an inlet dew point of 0.5°C
- Residuals dominated by *experimental* error in dew point sensors
- Model good enough to point out SLPM error
- Variability of testing conditions an issue
- Model has early temperature adsorption hump not seen in data
  - Not evident with higher flow rates or inlet dew points

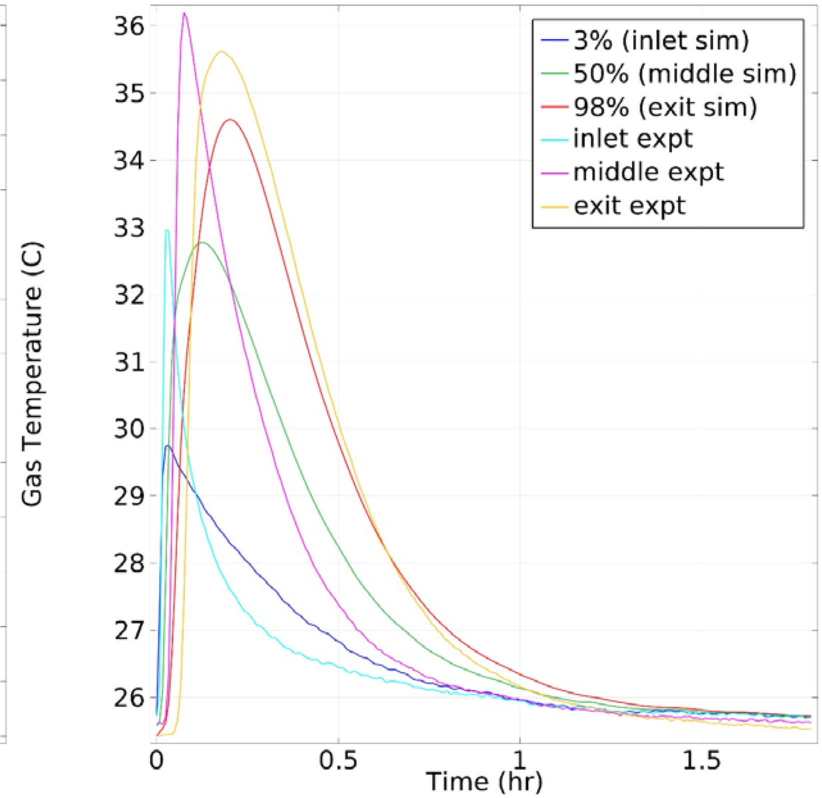




Example CO_2 5A CBT Results

- Carbon Dioxide on 5A zeolite RK38
- Flow is at 16 SLPM with an inlet partial vapor pressure of 5 Torr
- Consistently missing inlet sharp peak
- Temperature falloff and asymptotic behavior incorrect in models
- Excellent match to breakthrough curve





Summary

- Have constructed a *predictive* desiccant bed model
  - Applied to CBT
    - Various sorbates, sorbents, flow rates, concentrations
- Next: Generalize PDEs to 2D and 3D (!)
- Or: Use COMSOL modules
  - Velocity and pressure modules appropriate?
  - Have verified thermal modules give PDE results, but:
    - Assumption of $T_g \sim T_s$ not always valid
- Then: Apply same model methodology to CDRA Sorbent Beds
  - Complex 3D geometry
  - Including heaters
  - Uses vacuum desorption
  - Have to model H_2O/CO_2 sorption competition

→Full System Predictive CDRA Model!